

PROJECT NUMBER: 1754  
PROJECT TITLE : Spectroscopic Studies of Tobacco and Smoke Components  
PROJECT LEADER: W. N. Einolf  
PERIOD COVERED: September, 1985

NMR (J. Wooten, R. Bassfield, J. Campbell)

$^{13}\text{C}$  NMR was used to follow the appearance and disappearance of peaks in a cooked flavor reaction in a collaborative study with J. Lephardt. By adjusting the concentration of the reactants to control the rate of the reaction, the appearance of products and disappearance of reactants could be followed over a period of three days. Glucosylamine, diglucosylamine, fructose, glucose and fructosazines were monitored.<sup>4</sup>

The collaborative study (with G. Chan) of di-mannose compounds has been completed. Experiments involving elevated temperature and deuterium exchange did not clarify the region of 3.8-4.4ppm to make possible all proton assignments. However, the two compounds in question (the 2- and 3-substituted compounds reported last month) can be distinguished without these data.<sup>1</sup>

Since requests for two-dimensional NMR analyses have increased, additional experiments have been run on the XL-400 NMR. So far, only one, the carbon-carbon connectivity, does not work on this instrument.<sup>1,2</sup>

MS (D. Magin, W. N. Einolf)

A series of sclaral compounds have been submitted for GC/MS evaluation. These include isomers of sclaral, methyl, ethyl and isopropyl ethers, sclereolide, anhydrosclaral isomers, and sclaral phenethyl ether. The data are now being analyzed.<sup>3</sup>

We have received programs from D. Zayelski (USDA, North Dakota) which contain routines he uses to transfer files from one computer to another. We will use these programs in an attempt to transfer files between F. Hsu's data system and our SS-200. Ultimately, we hope to be able to link three data systems - F. Hsu's, our SS-200 and J. Naworal's - so that we can build a data base which will reside in the SS-200 memory.<sup>3</sup>

W. N. Einolf attended and presented a paper at the 10th International Mass Spectrometry Conference. A trip report has been written.<sup>5</sup>

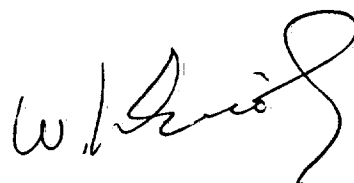
Additional cigarettes were made by D. Petri and are being conditioned. Another control LTF-IIA (new supplier of sodium polypectate and calcium lactate), and LTF-IIA with 10% DAP and 10% arbutin (hydroquinone- $\beta$ -D-glucopyranoside) have been made. The use of internal standards is also being evaluated.<sup>2</sup>

REFERENCES

1. R. Bassfield, N.B. 7398.
2. N. Einolf, N.B. 8040.

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3. D. Magin, N.B. 8222.
4. J. Wooten
5. W. N. Einolf, "Trip Report: 10th International Mass Spectrometry Conference", Memo to R. H. Cox, September 19, 1985.



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